

Myrcene

123-35-3 | DTXSID6025692

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

## Model Results

**Predicted value:** 3.07 mmHg

**Global applicability domain:** Inside

**Local applicability domain index:** 6.95e-01

**Confidence level:** 8.04e-01

## Nearest Neighbors from the Training Set

Image not found

Hydroquinone

**Measured:** 2.01

**Predicted:** 9.78e-05

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alpha-Bromotoluene

**Measured:** 15.7

**Predicted:** 4.50e-01

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2-Propanone, 1-chloro-1,1,3,3,3-pentafluoro-

**Measured:** 2.50

**Predicted:** 2670

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Dimethylamine

**Measured:** 2.93

**Predicted:** 664

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Benzene, 2-ethenyl-1,4-dimethyl-

**Measured:** 4.00

**Predicted:** 9.83e-01